New EOS for Mercury Vapor up to 1650 K and 130 MPa

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In the "Thermophysical Properties of Mercury", M.P. Vukalovich et. al, Moscow, 1971 give a vapor phase equation of state (EOS) and tables of the thermodynamic properties calculated up to 20 MPa. Now we have some new experimental data for mercury vapor: pVT-data (I.K. Kikoin, A.P.Senchenkov (1967); S.P. Naurzakov (1973); W.Goetzlaff (1988)), sound velocity (V.F. Kozhevnikov et al., (1999)). These new data and saturated vapor pressures Ps(T) (from the Gibbs equation G' (T,Ps) = G" (T, Hvap, Ps) up to 1650 K were simultaneously approximated by the: 1) weighted nonlinear least squares; 2) ES in the virial form with the 2d, 3d, 4th and 5th virial coefficients; 3) interatomic potential Lennard- Jones m-6 type with 3 parameters d, eps, m. Virial coefficients (for additive interatomic forces) we have from P.Reipert's dissertation (1978) for m=9,12 and 18.

The results are: 1) d = 2.78 /- 0.03 A, eps = 818.4 /- 50 K, m = 8.4 /- 0.6, Hvap(0 K)= 64530 /- 45 J/mol , and their error matrix; 2) new extended tables for the saturated and superheated vapor (Z, h,s,Cp,Cv, a and Ps-Ts (ordinary notations) up to 130 MPa. The main question is: from new spectroscopy data for Hg 2 we have eps < 550 K, why?